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Grinding Surface Creation Simulation using Finite Element Method and Molecular Dynamics

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Abstract. This paper presents some research results of the application of finite element method and molecular dynamics in the simulation of grinding surface creation. The comparison of these two methods shows that both methods could illustrate the material removal phenomena and provide useful information of grinding mechanics, but they have different feasible application arranges depending on the level of size scales. The investigation demonstrated that rubbing hypothesis of grinding material removal mechanism is valid at all size level even down to nanometre level. Further investigation areas are identified in the paper.

Introduction

Grinding is one of most commonly used material removal methods, which is applied to a wide range of applications from ultra-precision surface creation to extremely high speed material removal. Grinding is a very complicated process comparing to other machining process that uses geometrically defined cutting edges. Understand the material removal mechanism of grinding is a critical issue to define operational strategy for grinding process optimisation. Many researches have been undertaken in order to understand the material behaviours under different grinding conditions.

The finite element method (FEM) is the most frequently used numerical methods for metal cutting process analyses [1]. Due to the scale of grinding chip formation and the high speed of grinding, it is difficult to observe the material deformation and chip formation during grinding. The simulation of material processing using finite element method (FEM) is a convenient tool to illustrate the material behaviour during processing. However when the machining chip size becomes smaller, it is difficult and sometimes is impossible to use FEM to simulate the material removal. When the chip size is similar to molecule size, the assumption on FEM does not present the real situation. In such case, molecular dynamics (MD) analysis method could be an alternative method. With the increasing capability of computer, using Finite Element Method (FEM) and Molecular Dynamics (MD) for grinding simulation become feasible [2]. In this paper, grinding surface creation is investigated by using FEM and MD.

With FEM, grinding process has been modelled using heat transfer modelling technique in which case grinding wheel has been modelled as moving heat source and using elasto-mechanical material characteristic where the grinding wheel has been modelled as mechanical surface pressure [2-4]. This type of model is called as macro-scale model which deal with the interaction between grinding wheel and workpiece [2, 5]. The other approach is modelling of single grain action during machining process and called as micro-scale model dealing with individual grain interaction with workpiece [2, 5]. Micro-scale modelling of grinding is particularly suitable for simulation of grinding surface creation. However it is still in development stage due to the difficulty of FEM at the level of sub-micron level.

Micro-scale FEA model of grinding process was difficult because it requires high computational power. However, recently researchers have begun to investigate on micro-scale modelling and simulation of grinding process [2, 5, 6]. The grinding action of a single grain including rubbing,

ploughing and cutting three phases was first put forth by Hahn [7] and was called as a prevailing rubbing hypothesis [8]. Single grain scratch tests have been conducted to perform physical process experimentally. One of the earliest researches was performed by Takenaka using single grit action over the workpiece [9]. He verified the Hahn's rubbing hypothesis at the depth of cut about 0.5μm or less. All three grinding action described by Hahn, namely cutting, rubbing and ploughing processes were observed. He concluded that the rate of cutting process is relatively small and decreases with decrease of depth of cut, however, the rate of the ploughing process increase with decrease depth of cut.

Ram et al [10] developed a 2D simulation of an abrasive grain using elasticity theory. They mainly investigated the wear-induced elastic stresses due to impact and sliding of abrasive particle in tribological contact situation. They used Hertzian contact theory and LS-Dyna implicit finite element analysis to implement their model and their FE model agreed closely to the theoretical results. Yao et al [11] investigated the elastic contact of two dimensional rough surfaces by using multiscale finite element method. They concluded that Hertz theory is not fully capable to explain when approaching finer scale geometry. On the fine scale, the real contact traction at the peak of an asperity would be many times higher than the results of Hertz theory. Lambropoulos et al [12] developed a finite element model for axisymmetric indentation of glass surfaces. It was developed to study in plastic zones created by abrasive grain contact. Ohbuchi and Obikawa [13] revealed that upheaval or residual stock removal was caused by the effect of grain shape and cutting speed, and effect of elastic deformation of grain. Doman et al [8] developed a three dimensional FE model of rubbing and ploughing phases in single-grain grinding considering elastoplastic material characteristic. Scratch test was used to validate the model and very good agreement was obtained with simulation. Klocke et al [14] used FEM to simulate the single-grit abrasive process on the workpiece, where a single-grit scratch was modelled as a 2D considering thermostructural material properties and DEFORM was used as a simulation environment.

The use of Molecular Dynamics (MD) simulation may prove to be an effective way for the analysis and prediction of machining processes at the nanometre scale. The MD method can improve our understanding of nanometric processes and subsequently give helpful insights into phenomena that are otherwise intractable to investigate experimentally. In the field of nanometric cutting, Belak pioneered work on the study of cutting copper with a diamond tool [15]. Initially, the method was used extensively to model indentation and cutting. In 1991, Belak and Stowers [16] first applied the MD to abrasive processes and Rentsch and Inasaki's study [17] later presented the first results of simulations targeted on the pile-up phenomenon in abrasive machining. Komanduri et al [18] investigated the effect of tool geometry in nanometric cutting. They considered indentation sliding to simulate the ultraprecision machining, grinding and abrasion. Results showed that with different tool radii, the cutting force increased with depth of cut and was independent from the (d/r) ratio. Also, the specify energy increased rapidly with decrease in depth of cut. They proposed that for grinding of ductile materials, the appropriate model would be machining using tools of either large radii relative to the depth of cut or large negative rake angle. Komanduri et al study was focused on pointed tools with various radii, but abrasive grains could be of different and complex shapes, which require that various tool end shapes should be investigated for practical realism.

Grinding Surface Creation Simulation Using Finite Element Method

In the FEM model of grinding surface creation, re-meshing technique is used to control distortion of element due to dramatically increasing strain rate at large deformation state such as grinding. Fine meshes over the cutting area also provide better conformity of contact between grain and workpiece. Material properties of grain and workpiece used in simulation are shown in Table 1. Grain is modelled as half solid sphere with a diameter of 100 μm. The length, width and depth of the workpiece are 2 mm, 1 mm and 0.5 mm respectively. The grinding path of single grain for FEM

simulation is illustrated in Fig. 1. In this research, FEM simulation of a single grain machining is conducted by using commercial software package of ABAQUS/CAE.

Table 1. Material properties of grain and workpiece

Grain			**Workpiece**		
Mass density (kg/ m^3)	4000		7800		
Young's modulus (GPa)	530		200		
Poisson's ratio	0.2		0.3		
Plastic Properties			**Plastic Properties**		
	Yield stress (Gpa)	Plastic strain rate		Yield stress (MPa)	Plastic strain rate
1	15	0	1	180	0
2	15.4	0.03	2	200	0.1
3	16	0.2	3	250	0.25
4	16.5	0.5	4	300	0.3

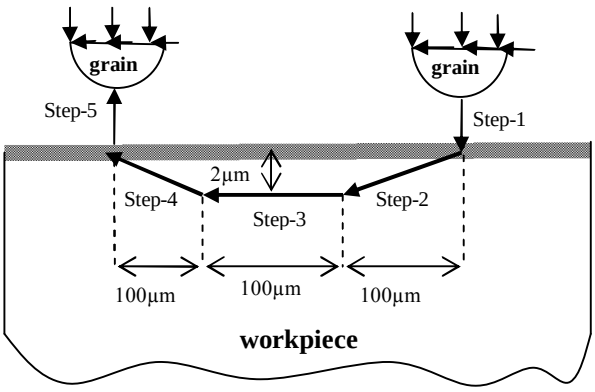


Fig. 1. A single grain path in simulation

A typical mesh of the grain and workpiece is C3D4 element which is a four node linear tetrahedron elements are used to mesh both single grain and workpiece part. Both parts are meshed by using free-mesh technique in first stage. Coarse meshing may result in poor conformity of simulation due to the relatively large stress gradients in the grinding contact zone. Re-meshing rules are applied to improve conformity. Encastre (all translational and rotational degree of freedom are fixed) boundary conditions is applied to workpiece bottom plane nodes. A two directional, -Z and -X, displacement boundary condition is applied to the nodes on grain top flat surface to simulate indentation and sliding respectively. Boundary conditions are created in the first step and propagated through all steps. Displacement boundary conditions are modified according to the grain simulation path.

Fig. 2 shows the deformation and stress distribution in the workpiece along cutting path. The largest depth represents the grain position during simulation, which includes elastic and plastic deformation. The residual deformation represents plastic deformation. Workpiece material in front of grain is agglomerated as the beginning stage of chip formation. When the stresses reach the breaking point, chips may form. Stresses due to elastic deformation are removed from workpiece and only residuals due to plastic deformation remain on the workpiece.

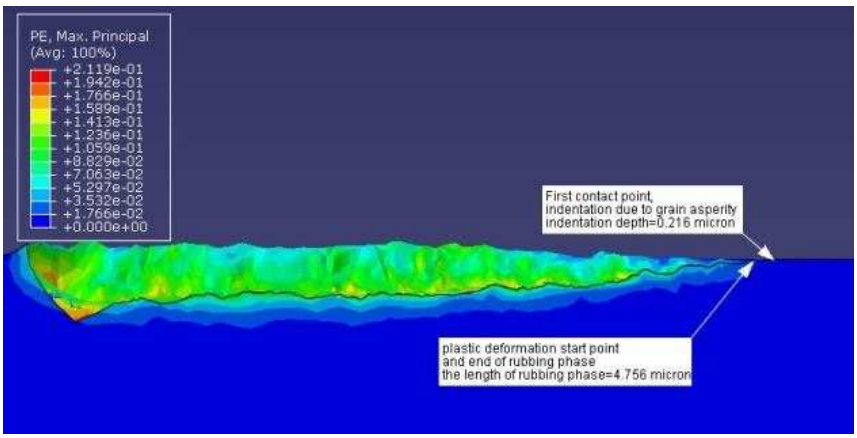


Fig.2 Stress and deformation of rubbing and ploughing phase in a grinding simulation

Rubbing, ploughing and chip formation are the three phases taken place during grinding process. Rubbing phase only include elastic deformation while ploughing phase include elastic and plastic deformation together. Transformation from rubbing to ploughing phase presents at the beginning of simulation process, a very small stress-free field can be attributed to rubbing phase. The rubbing

length is measured as a 4.756 µm. In ploughing phase residual stresses exists due to plastic deformation in the workpiece.

A simulation is designed to demonstrate how ploughing could affect the generation of ground surface in grinding, where a single grain scratches the workpiece three times with 10 µm feed in transverse direction. Fig. 3 shows subsequent grit passes push material aside forming ridges which alter the ground surface. The subsequent scratches give larger depths of cut and the grove shape becomes unsymmetrical. Even so, the force of each pass presents similar feature as shown in Fig. 4.

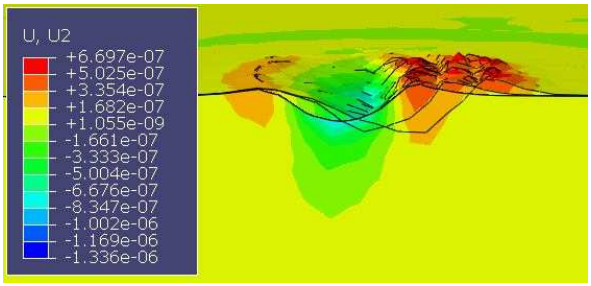


Fig. 3. The deformation presented after 3 parallel scratch passes with 10 µm apart

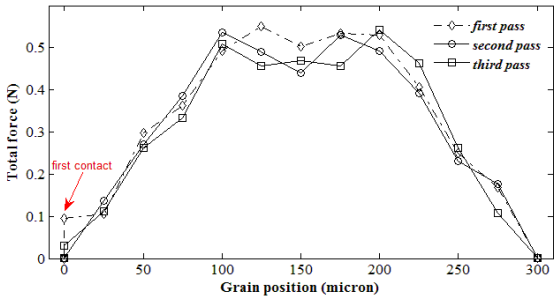
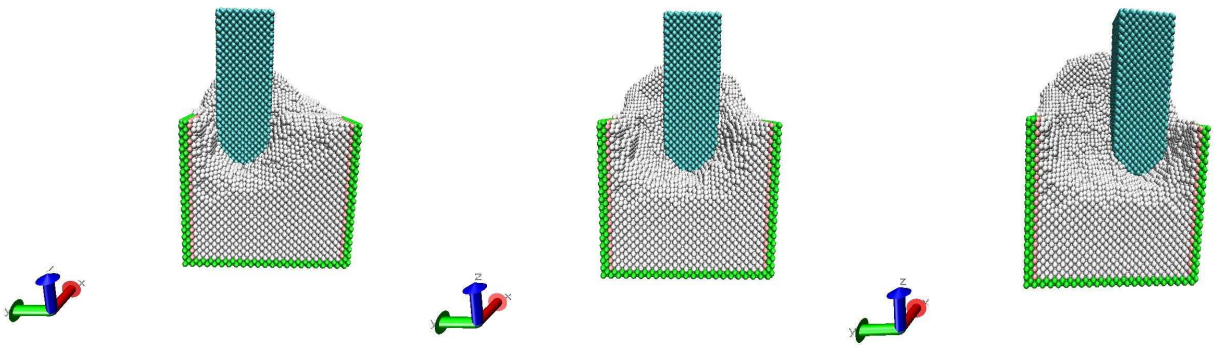


Fig. 4. Force variation in the parallel scratching tests

Grinding Surface Creation Simulation Using Molecular Dynamics

The nanometric cutting model consists of a monocrystalline copper workpiece and a diamond tool. The model configuration has a total of 54232 atoms. The workpiece is made up of 43240 copper atoms with the face-centred cubic (fcc) lattice. It includes 3 kinds of atoms namely; boundary atoms, thermostat atoms and Newtonian atoms. The cutting tool has 10992 carbon atoms with diamond lattice structure. It has been previously established that the EAM potential is very suitable for the Cu-Cu interactions [19-20], the Morse potential is a good choice for the Cu-C interactions [21] and Tersoff Potential is chosen for the C-C interactions [22].

The simulation conditions applied in this study are the following, viz: bulk temperature is 293K, the cutting direction is along the x-axis, the cutting speed is 150m/s, the cross feed is 1.5nm in transverse direction, the time step is 0.3fs and the simulation run is 150000 steps. The cutting tool is fairly pointed shaped. For the workpiece, the boundary atoms are kept fixed to reduce edge effects. The thermostat atoms conduct the heat generated during the cutting process out of the cutting region. This is achieved by the velocity scaling of the thermostat atoms with the conversion between the kinetic energy (KE) and temperature. The Newtonian atoms obey the Newton's equation of motion. The depths of cut used in the study are 0.5nm, 1.0nm, 1.5nm, 2nm, 2.5nm and 3 nm. The LAMMPS parallel MD software [23] was used for the simulations. The VMD software [24] was used for the visualization of the results. Fig. 5 illustrates the simulation results of multiple cutting passes, where the smaller scale of ploughing ridges can be found on the created surface.



First pass Second pass Third pass

Fig. 5. Surface creation simulation by molecular dynamics

Fig. 6 shows the stress variation with depth of cut for the three passes. It can be observed that as the depth of cut increases, the stress values decrease and the forces are higher for passes 2 and 3. The stress values are in the range from 20 GPa to 160 GPa. The value remains constant at around 20 GPa for all passes for higher depth of cut – from 2.5nm. The highest stress values are for depth of cut of 0.5nm during passes 2 and 3.

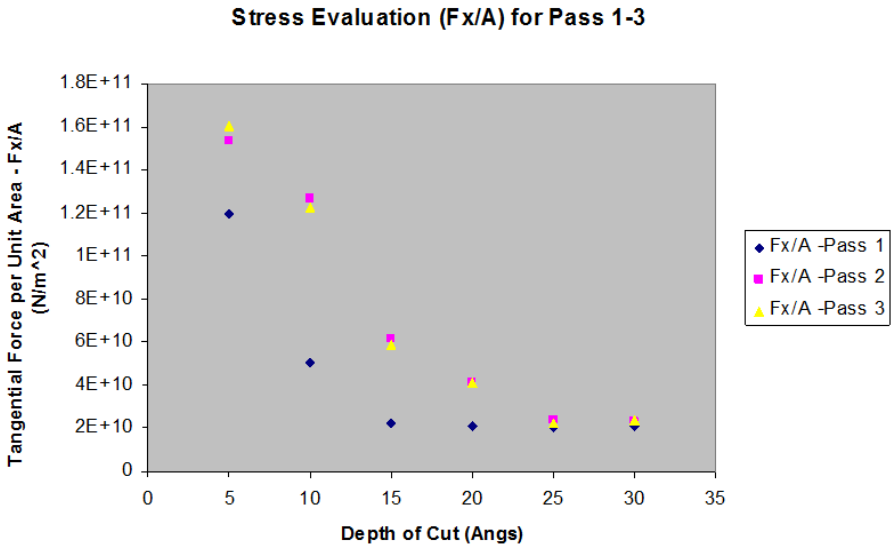


Fig. 6. The variation of cutting stress under different depth of cut

Discussion and Conclusion

It has been demonstrated that the grinding surface creation can be visualised by applying FEM and MD. With micro-scale modelling approaches, the basic grinding material removal mechanism, rubbing, ploughing and cutting, can be studied and illustrated. The grinding-induced forces and stresses, geometrical ground surface formation can be investigated by varying different conditions at different scale levels. Using a commercial software package of ABAQUS/CAE for FEM simulation, the rubbing and ploughing phenomena of single grain machining has been successfully illustrated in 3D models. However, the cutting phenomenon is still difficult to fulfil, because of the extremely high distortion within grinding zone under high rake angle of the grain. Other commercial softwares, commonly used for cutting simulation, also present the same difficulty when the simulation is carried out under less than a micron level. Therefore, for abrasive machining simulation at nanometre level, MD method is recommended for the study of surface creation. However, the power of computing and simulation time could be an obstacle for its application due to the size of molecule.

The results of FEM simulation provide essential information about grinding process, including stress distribution and surface formation during grinding. Ploughing and rubbing phase can be observed clearly as well as ridge formation. Force variation in the grinding depends on grit cutting path. The material bulged due to previous ploughing action will increase cutting forces in subsequent cutting passes. As for FEM model, re-meshing strategy is very essential to obtain reliable result. It provides very fine size meshes through contact area to alleviate the element distortion due to large plastic deformation. With the aid of simulations, some physical parameters, such as force, can be quantitatively analysed. Moreover, ground surface roughness and material removal characteristics can also be studied by using properly designed FEM model. It is interesting to note that the cutting forces remain almost the same in a series of overlap cuttings in the results of FEM analysis, while the force results from MD show a step increase when the depth of cut is less than 2 nm. This phenomenon may be related to the cutting edge shape and cutting size-effects. Significant cutting size-effects are found at nanometre level. Further investigation in this area is required.

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